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On Coulomb wave functions

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Abstract. The irregular radial Coulomb wave function in repulsive fields is expressed, for any angular momentum value, in series of Bessel functions of arbitrary order. Previous expansions, obtained for angular momenta zero and one, can now be obtained as special cases. The expansion can be most conveniently used for high-energy particles.

1. *The Coulomb wave functions.* The radial equation which describes the relative motion of two positively charged particles interacting through their Coulomb fields is

$$\frac{d^2\chi}{dr^2}+\left\{\frac{2\mu}{\hbar^2}\left(E-\frac{ZZ'e^2}{r}\right)-\frac{L(L+1)}{r^2}\right\}\chi=0, \tag{1}$$

where χ is r times the radial factor of the wave function, L is the orbital angular momentum, μ is the reduced mass, r is the distance between the two particles, Ze, $Z'e$ are their charges and E is the energy associated with the relative motion. By the substitutions

$$E=\frac{\mu Z^2Z'^2e^4}{2\hbar^2\eta^2}, \quad r=\frac{\hbar^2\eta\rho}{\mu ZZ'e^2}, \tag{2}$$

this equation transforms into

$$\frac{d^2\chi}{d\rho^2}+\left\{1-\frac{2\eta}{\rho}-\frac{L(L+1)}{\rho^2}\right\}\chi=0, \tag{3}$$

which is a special form of the confluent hypergeometric equation. In the notation of Whittaker and Watson (1), two fundamental solutions of this equation are $M_{i\eta,L+\frac{1}{2}}(2i\rho)$ and $W_{i\eta,L+\frac{1}{2}}(2i\rho)$. If Coulomb's law applies for all values of r then one needs only the regular solution $M_{i\eta,L+\frac{1}{2}}(2i\rho)$. In the usual discussions of nuclear collisions, however, one has to suppose that the repulsive Coulomb field is modified at distances comparable with or smaller than nuclear dimensions. In these cases one needs the regular as well as the irregular solutions of (3). In standard notations (2), the normalized forms of these solutions can be expressed in terms of Whittaker's functions by the equations (3)

$$F_L(\eta,\rho)=\tfrac{1}{2}C_L(\eta)\,(i)^{-L-1}\,M_{i\eta,L+\frac{1}{2}}(2i\rho), \tag{4}$$

$$G_L(\eta,\rho)=\frac{1}{(2L+1)!\,C_L(\eta)}\,\Re(\Gamma(L+1-i\eta)\,(i)^L\,W_{i\eta,L+\frac{1}{2}}(2i\rho)), \tag{5}$$

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where $\Re$ stands for the real part and

$$C_L(\eta) = \frac{1}{(2L+1)!}\left\{(1^2+\eta^2)(2^2+\eta^2)\dots(L^2+\eta^2)\frac{2\pi\eta}{e^{2\pi\eta}-1}\right\}^{\frac{1}{2}}. \tag{6}$$

In various problems, the functions F_L and G_L are conveniently represented by expansions in series of Bessel functions. For low-energy particles, expansions for both F_L and G_L had been developed ((4), (5), (6)). In the case of high-energy particles, expansions had been obtained for F_L for all L ((2), (6), (7), (8)), and for G_L in the cases of $L = 0$ and 1 only (9). We shall now develop, for high-energy particles, a Bessel-function expansion of G_L for all L.

2. *Expansion of* $W_{k,m}(z)$. This function can be expressed ((10), (11)), when $2m$ is an integer or zero, by the equation

$$W_{k,m}(z) = \frac{(-)^{2m+1}}{2\Gamma(\frac{1}{2}-m-k)}\{\psi(\tfrac{1}{2}+m-k)+\psi(\tfrac{1}{2}-m-k)\}I_{k,m}(z)$$
$$+\tfrac{1}{2}(-)^{2m+1}\left\{\frac{1}{\Gamma(\frac{1}{2}-m-k)}\frac{\partial}{\partial m}I_{k,m}(z)-\frac{1}{\Gamma(\frac{1}{2}+m-k)}\frac{\partial}{\partial m}I_{k,-m}(z)\right\}, \tag{7}$$

where
$$I_{k,m}(z) = \frac{1}{\Gamma(1+2m)}M_{k,m}(z), \tag{8}$$

ψ is the logarithmic derivative of the gamma-function and $2m$ is made an integer after differentiation. In a previous paper (8), an expansion of the function $M_{k,m}(z)$ in a series of Bessel functions of arbitrary order was obtained. From that expansion and (8) we have

$$I_{k,m}(z) = \frac{4^\lambda\Gamma(\lambda+1)}{\Gamma(2m+1)}z^{\frac{1}{2}+m-\lambda}\sum_{n=0}^{\infty}\frac{A^\lambda_{m,n}(k)}{(2m+1)_n}I_{\lambda+n}(\tfrac{1}{2}z), \tag{9}$$

where λ is arbitrary and

$$A^\lambda_{m,n}(k) = (-)^n\frac{(2\lambda-2m)_n(2\lambda)_n(\lambda+n)}{n!(\lambda)}{}_3F_2\left[\begin{matrix}-n, \lambda-m-k, 2\lambda+n;\\ 2\lambda-2m, \lambda+\frac{1}{2};\end{matrix}1\right] \tag{10}$$

or, alternatively,
$$A^\lambda_{m,0} = 1, \quad A^\lambda_{m,1} = -4k(\lambda+1),$$

$$\frac{n}{\lambda+n}A^\lambda_{m,n} = -4kA^\lambda_{m,n-1}+\frac{(2m+n-1)(2\lambda+n-2)(2\lambda-2m+n-2)}{\lambda+n-2}A^\lambda_{m,n-2}. \tag{11}$$

The expansion (9) is valid when λ is not a negative integer and is uniformly convergent for all finite values of z and for any finite values of the parameters.

If we differentiate (9) with respect to m and then replace λ by $\lambda+2m$, we obtain

$$\frac{\partial}{\partial m}\{I_{k,m}(z)\} = (\log z - 2\psi(2m+1))I_{k,m}(z)$$
$$+\frac{4^{\lambda+2m}\Gamma(\lambda+2m+1)}{\Gamma(2m+1)}z^{\frac{1}{2}-m-\lambda}\sum_{n=0}^{\infty}\left\{\frac{\partial}{\partial m}\left(\frac{A^\mu_{m,n}(k)}{(2m+1)_n}\right)\right\}_{\mu=\lambda+2m}I_{\lambda+2m+n}(\tfrac{1}{2}z). \tag{12}$$

Again, if we change the sign of m in (9) and differentiate with respect to m, using the equation

$$I_{k,-m}(z) = (-)^{2m}\frac{\Gamma(\frac{1}{2}+m+k)}{\Gamma(\frac{1}{2}-m+k)}I_{k,m}(z),$$

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where $2m$ is an integer, we obtain

$$\frac{\partial}{\partial m}\{I_{k,-m}(z)\} = (-)^{2m+1}\frac{\Gamma(\frac{1}{2}+m+k)}{\Gamma(\frac{1}{2}-m+k)}(\log z+2\gamma-2C)\,I_{k,m}(z)$$
$$+2(-)^{2m}4^{\lambda}\Gamma(\lambda+1)\,z^{\frac{1}{2}-m-\lambda}\sum_{n=0}^{2m-1}(-)^n\,\Gamma(2m-n)\,A^{\lambda}_{-m,n}(k)\,I_{\lambda+n}(\tfrac{1}{2}z)$$
$$+4^{\lambda}\Gamma(\lambda+1)\,z^{\frac{1}{2}-m-\lambda}\sum_{n=2m}^{\infty}\left(\frac{\partial}{\partial m}(A^{\lambda}_{-m,n}(k))\right.$$
$$\left.+2A^{\lambda}_{-m,n}(k)\,(\psi(-2m+1+n)-\psi(1)-C)\right)\frac{I_{\lambda+n}(\frac{1}{2}z)}{\Gamma(-2m+1+n)}, \quad (13)$$

where γ is Euler's constant and C is an arbitrary constant, independent of n and z, which has been introduced for convenience.

If we insert (12) and (13) in (7), we obtain

$$W_{k,m}(z) = \frac{(-)^{2m+1}}{\Gamma(\frac{1}{2}-m-k)}\{\log z+\tfrac{1}{2}\psi(\tfrac{1}{2}+m-k)+\tfrac{1}{2}\psi(\tfrac{1}{2}-m-k)-\psi(2m+1)+\gamma-C\}\,I_{k,m}(z)$$
$$+\frac{4^{\lambda}\Gamma(\lambda+1)}{\Gamma(\frac{1}{2}+m-k)}\,z^{\frac{1}{2}-m-\lambda}\sum_{n=0}^{2m-1}(-)^n\,\Gamma(2m-n)\,A^{\lambda}_{-m,n}(k)\,I_{\lambda+n}(\tfrac{1}{2}z)$$
$$+\frac{(-)^{2m+1}\,4^{\lambda+2m}\Gamma(\lambda+2m+1)}{2\Gamma(2m+1)\,\Gamma(\frac{1}{2}-m-k)}\,z^{\frac{1}{2}-m-\lambda}\sum_{n=0}^{\infty}\left\{\frac{\partial}{\partial m}\left(\frac{A^{\mu}_{m,n}(k)}{(2m+1)_n}\right)\right\}_{\mu=\lambda+2m}I_{\lambda+2m+n}(\tfrac{1}{2}z)$$
$$+\frac{(-)^{2m}\,4^{\lambda}\Gamma(\lambda+1)}{2\Gamma(\frac{1}{2}+m-k)}\,z^{\frac{1}{2}-m-\lambda}\sum_{n=2m}^{\infty}\left\{\frac{\partial}{\partial m}(A^{\lambda}_{-m,n}(k))\right.$$
$$\left.+2A^{\lambda}_{-m,n}(k)\,(\psi(-2m+1+n)-\psi(1)-C)\right\}\frac{I_{\lambda+n}(\frac{1}{2}z)}{\Gamma(-2m+1+n)}. \quad (14)$$

For convenience, we choose C so that the coefficient of $I_{\lambda+2m}(\frac{1}{2}z)$ in the series on the right-hand side of this equation is zero. The required value of C, as seen from (14), is given by

$$C = \frac{1}{2}\left(\frac{1}{A^{\lambda}_{-m,n}}\frac{\partial}{\partial m}A^{\lambda}_{-m,n}\right)_{n=2m}.$$

To evaluate this expression, we change the sign of m in (10) and apply the following transformation formula ((12), § 3·8, (1))

$${}_3F_2\left[\begin{matrix}-n,\alpha_1,\alpha_2;\\ \beta_1,\beta_2;\end{matrix}\;1\right] = \frac{(\beta_1-\alpha_1)_n}{(\beta_1)_n}\,{}_3F_2\left[\begin{matrix}-n,\alpha_1,\beta_2-\alpha_2;\\ -n+\alpha_1-\beta_1+1,\beta_2;\end{matrix}\;1\right]$$

to obtain

$$A^{\lambda}_{-m,n}(k) = \frac{(-)^n\,(2\lambda+2m)_n\,(\frac{1}{2}-m+k)_n\,(2\lambda)_n\,(\lambda+n)}{n!\,(\lambda+\frac{1}{2})_n\,(\lambda)}\,{}_3F_2\left[\begin{matrix}-n,\lambda+m-k,2m-n;\\ -n+m-k+\frac{1}{2},2\lambda+2m;\end{matrix}\;1\right].$$

Taking the logarithmic derivative of this equation with respect to m and then putting $n = 2m$, it follows that

$$C = \psi(2\lambda+4m)-\psi(2\lambda+2m)-\tfrac{1}{2}\psi(\tfrac{1}{2}+m+k)$$
$$+\tfrac{1}{2}\psi(\tfrac{1}{2}-m+k)+\sum_{r=1}^{2m}\frac{(-2m)_r\,(\lambda+m-k)_r}{r(\frac{1}{2}-m-k)_r\,(2\lambda+2m)_r}.$$

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Inserting this value of C in (14), and the values of the expressions

$$\left\{\frac{\partial}{\partial m}\left(\frac{A^{\mu}_{m,n}(k)}{(2m+1)_n}\right)\right\}_{\mu=\lambda+2m} \quad \text{and} \quad \frac{\partial}{\partial m}(A^{\lambda}_{-m,n}(k)),$$

as obtained from (10), we get

$$\begin{aligned} W_{k,m}(z) = \frac{(-)^{2m+1}}{\Gamma(\frac{1}{2}-m-k)}\Big\{&\log z + \psi(\tfrac{1}{2}-m-k) - \psi(2m+1) \\ &+ \gamma - \psi(2\lambda+4m) + \psi(2\lambda+2m) - \sum_{r=1}^{2m} \frac{(-2m)_r\,(\lambda+m-k)_r}{r!\,(\tfrac{1}{2}-m-k)_r\,(2\lambda+2m)_r}\Big\} I_{k,m}(z) \\ &+ \frac{4^{\lambda}\Gamma(\lambda+1)\,\Gamma(2m)}{\Gamma(\frac{1}{2}+m-k)}\, z^{\frac{1}{2}-m-\lambda} \sum_{n=0}^{\infty} b^{\lambda}_{m,n}(k)\, I_{\lambda+n}(\tfrac{1}{2}z), \end{aligned} \tag{15}$$

where

$$\begin{aligned} b^{\lambda}_{m,n}(k) &= \frac{(-)^n}{(2m-n)_n} A^{\lambda}_{-m,n}(k) \quad \text{for} \quad 0 \leqslant n < 2m, \\ &= 0 \quad \text{for} \quad n = 2m, \\ &= \frac{(-)^n\, 4^{2m}(\lambda+1)_{2m}\,(\frac{1}{2}-m-k)_{2m}\,(2\lambda+2m)_n\,(2\lambda)_n\,(\lambda+n)}{n!\,(n-2m)!\,(2m-1)!\,(2\lambda)_{4m+1}} \\ &\quad \times \Big\{ \sum_{r=0}^{n-2m} \frac{(2m-n)_r\,(\lambda+m-k)_r\,(2\lambda+2m+n)_r}{r!\,(2\lambda+2m)_r\,(\lambda+2m)_r} \\ &\quad \times \big(2\phi(2\lambda+2m+r, n-r-2m) + 2\phi(2m+1, n-2m) + \phi(\lambda+m-k, r)\big)\Big\} \\ &\quad + \frac{(-)^{n+2m}(2\lambda)_n\,(2\lambda+2m)_n\,(\frac{1}{2}-m+k)_n\,(\lambda+n)}{n!\,(2m-1)!\,(\lambda+\frac{1}{2})_n\,(2\lambda)} \\ &\quad \times \Big\{ \sum_{r=0}^{n} \frac{(-n)_r\,(\lambda+m-k)_r\,(2m-n)_r}{r!\,(-n+m-k+\frac{1}{2})_r\,(2\lambda+2m)_r} \Big(2\phi(2\lambda+2m+r, n-r) + 2\phi(2m-n, r) \\ &\quad - \phi(\tfrac{1}{2}+m+k, n-2m) + \phi(\lambda+m-k, r) + 2\phi(1, n-2m) - 2\phi(2\lambda+2m, 2m) \\ &\quad - 2\sum_{\nu=1}^{2m} \frac{(-2m)_\nu\,(\lambda+m-k)_\nu}{\nu\,(-n+m-k+\frac{1}{2})_\nu\,(2\lambda+2m)_\nu}\Big)\Big\} \quad \text{for} \quad n > 2m, \end{aligned} \tag{16}$$

where $\phi(\alpha, n)$ denotes $\qquad \phi(\alpha, n) = \psi(\alpha+n) - \psi(\alpha).$

The expansion (15) expresses the Whittaker function $W_{k,m}(z)$ in a series of Bessel functions of arbitrary order when $2m$ is an integer or zero. The expansion coefficients, as given in (16), are rather involved. However, they can be presented in a convenient way for computation by means of a recurrence relation. This is obtained by substituting (15) in the differential equation satisfied by $W_{k,m}(z)$ and replacing $I_{k,m}(z)$ by its expansion in series of Bessel functions as given by (9) with λ replaced by $\lambda+2m$. We then employ the recurrence formulae for the modified Bessel functions of the first kind and equate to zero the coefficient of $I_{\lambda+n}(\frac{1}{2}z)$, and thus obtain

$$\begin{aligned} &\frac{n(n-2m)}{n+\lambda} b^{\lambda}_{m,n} + 4k b^{\lambda}_{m,n-1} - \frac{(n+2\lambda-2)\,(n+2\lambda+2m-2)}{n+\lambda-2} b^{\lambda}_{m,n-2} \\ &\quad = \frac{2^{4m+1}(\frac{1}{2}-m+k)_{2m}\,(\lambda+1)_{2m}}{\Gamma(2m)\,\Gamma(2m+1)} \Big\{ \frac{n-m}{n+\lambda} a^{\lambda}_{m,n-2m} + \frac{n+m+2\lambda-2}{n+\lambda-2} a^{\lambda}_{m,n-2m-2} \Big\}, \end{aligned} \tag{17}$$

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where $$a^{\lambda}_{m,n}(k) = \frac{1}{(2m+1)_n} A^{\lambda+2m}_{m,n}(k),$$

and, from (11), has the values

$$a^{\lambda}_{m,0} = 1, \quad a^{\lambda}_{m,1} = -4k(\lambda+2m+1)/(2m+1),$$

$$\frac{n(n+2m)}{n+\lambda+2m} a^{\lambda}_{m,n} = -4k a^{\lambda}_{m,n-1} + \frac{(n+2\lambda+4m-2)(n+2\lambda+2m-2)}{n+\lambda+2m-2} a^{\lambda}_{m,n-2}. \tag{18}$$

Notice that in (17), $b^{\lambda}_{m,0} = 1$, $b^{\lambda}_{m,2m} = 0$ and $a^{\lambda}_{m,n} = 0$ for $n < 0$. In (15), λ should not be a negative integer. The expansion corresponding to (15), of $I_{k,m}(z)$ is

$$I_{k,m}(z) = \frac{4^{\lambda+2m}\Gamma(\lambda+2m+1)}{\Gamma(2m+1)} z^{\frac{1}{2}-m-\lambda} \sum_{n=1}^{\infty} a^{\lambda}_{m,n}(k) I_{\lambda+2m+n}(\tfrac{1}{2}z). \tag{19}$$

3. *Expansions of the wave functions.* Expansions of the irregular wave functions $G_L(\eta,\rho)$ in terms of Bessel functions may now be obtained from the expansion (15) of the Whittaker function $W_{k,m}(z)$. As seen from (17) and (18), the coefficients of the expansion of $G_L(\eta,\rho)$ will depend on those of the corresponding expansion of $F_L(\eta,\rho)$ obtainable from (19), so that both F_L and G_L may be computed at the same time. Substituting from (8) and (19) in (4) and making use of (18), we have

$$F_L(\eta,\rho) = 2^{3L+\lambda+1} C_L(\eta)\, \Gamma(\lambda+2L+2)\, \rho^{-L-\lambda} \sum_{n=0}^{\infty} P^{\lambda}_{L,n}(\eta)\, J_{2L+\lambda+n+1}(\rho), \tag{20}$$

where $J_r(\rho)$ is the Bessel function of the first kind and

$$P^{\lambda}_{L,0} = 1, \quad P^{\lambda}_{L,1} = 2\eta(2L+\lambda+2)/(L+1),$$

$$nP^{\lambda}_{L,n} = \frac{n+2L+\lambda+1}{n+2L+1}\left\{4\eta P^{\lambda}_{L,n-1} - \frac{(n+2\lambda+4L)(n+2\lambda+2L-1)}{n+2L+\lambda-1} P^{\lambda}_{L,n-2}\right\}. \tag{21}$$

Also, substituting from (15) in (5) and making use of (17), (18) and (21), we get

$$\begin{aligned} G_L(\eta,\rho) = \frac{2\eta}{C_0^2(\eta)}\Bigg\{&\log(2\rho) + \gamma - \psi(2L+2) - \psi(2\lambda+4L+2) + \psi(2\lambda+2L+1) \\ &+ \Re\psi(i\eta-L) - \Re\left(\sum_{r=1}^{2L+1} \frac{(-2L-1)_r (L+\lambda+\frac{1}{2}-i\eta)_r}{r(-i\eta-L)_r (2\lambda+2L+1)_r}\right)\Bigg\} F_L(\eta,\rho) \\ &+ \frac{4^{\lambda}\Gamma(\lambda+1)}{(2L+1)\, C_L(\eta)} (2\rho)^{-\lambda-L} \sum_{n=0}^{\infty} q^{\lambda}_{L,n}(\eta)\, J_{\lambda+n}(\rho), \end{aligned} \tag{22}$$

where $$q^{\lambda}_{L,0} = 1, \quad q^{\lambda}_{L,2L+1} = 0,$$

$$\begin{aligned} &\frac{n(n-2L-1)}{n+\lambda} q^{\lambda}_{L,n} - 4\eta q^{\lambda}_{L,n-1} + \frac{(n+2\lambda-2)(n+2\lambda+2L-1)}{n+\lambda-2} q^{\lambda}_{L,n-2} \\ &\quad = -4^{2L+1}(2L+1)(\lambda+1)_{2L+1} \frac{\eta C_L^2}{C_0^2} \\ &\qquad \times \left\{\frac{2n-2L-1}{n+\lambda} P^{\lambda}_{L,n-2L-1} - \frac{2n+2L+4\lambda-3}{n+\lambda-2} P^{\lambda}_{L,n-2L-3}\right\}. \end{aligned} \tag{23}$$

Notice that in (23), $P^{\lambda}_{L,n} = 0$ for $n < 0$. The special cases of (22) in which $\lambda = \frac{1}{2}$ and $L = 0$ or 1 correspond to those obtained previously by one of the authors (9). The

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expansion coefficients were, however, presented in a different way which can be deduced from (21) and (23) in these special cases.

The expansions (20) and (22) are practically useful for the computation of the wave functions for all values of ρ. The freedom in the choice of the order of the Bessel functions can be used to select expansions which suit the available tables of Bessel functions. As may be seen from (21) and (23), the expansions should be convenient for small or moderate values of η, that is for high or moderate energies.

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